

Shrinking stacking fault through glide of the Shockley partial dislocation in hard-sphere crystal under gravity

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Disappearance of a stacking fault in the hard-sphere crystal under gravity, such as reported by Zhu *et al.* [*Nature* **387** (1997) 883], has successfully been demonstrated by Monte Carlo simulations. We previously found that a less ordered (or defective) crystal formed above a bottom ordered crystal under stepwise controlled gravity [Mori *et al.* *J. Chem. Phys.* **124** (2006) 174507]. A defect in the upper defective region has been identified with a stacking fault for the (001) growth. We have looked at the shrinking of a stacking fault mediated by the motion of the Shockley partial dislocation; the Shockley partial dislocation terminating the lower end of the stacking fault glides. In addition, the presence of crystal strain, which cooperates with gravity to reduce stacking faults, has been observed.

Keywords: Hard spheres, colloidal crystal, gravity, sedimentation, stacking fault, Shockley partial dislocation, glide, Monte Carlo simulation

1 Introduction

The existence of a crystal-fluid phase transition in the hard-sphere (HS) system was observed in 1957 using both molecular dynamics (MD) [1] and Monte Carlo (MC) simulation techniques [2]. In the HS system the phase behaviour is governed by the particle number density only; the disordered fluid phase crystallizes into a face-centred cubic (fcc) crystal over a coexistence interval $0.494 < \phi < 0.545$ [3]^{||}, where $\phi = (\pi/6)\sigma^3(N/V)$ is the volume fraction of the HSs. Here, σ is the HS diameter, N the number of particles, and V the volume of the system. The HS system is often utilized as a model for colloids [5]. In order for colloidal crystals to have application as photonic crystals [6, 7, 8], it is important that the number of defects, such as

stacking faults, be reduced. However, the number of stacking faults present in a HS crystal is difficult to reduce, because the stacking disorder does not change the density. Indeed, the entropy difference between fcc and hexagonal close-packed (hcp) HS crystals has been calculated [9, 10, 11, 12, 13] and is, at most, of the order of $10^{-3}k_B$ per particle, where k_B is Boltzmann's constant. On the other hand, the density gradients induced by gravity have been observed to enhance colloidal crystallization. For example, HS-like suspensions, such as poly(methylmethacrylate) (PMMA) microparticles dispersed in a hydrocarbon medium as well as charge stabilized colloidal suspensions, have been seen to crystallize by sedimentation [14].

Interestingly, the 1997 experiment of Zhu *et al.* [15] suggests that stacking faults in HS suspensions were controlled by gravity. In this paper, we focus on the mechanism of the reduction of the stacking faults in colloidal crystals due to gravity. The conclusion of Zhu *et al.* is as follows: Whereas the resulting HS crystalline structure under microgravity on the Space Shuttle was observed to be random hexagonal-close-packed

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^{||} By adjusting the lateral box size so as to remove the stress of the crystal the coexistence region has been corrected slightly, i.e., $0.491 < \phi < 0.542$ [4]. However, the result has not been affected; the stress cannot be removed entirely because the system is nonuniform and, in addition, the crystal can rotate about z axis

(rhcp) [15], on Earth a mixture fcc and rhcp can be obtained [16]. The results of the experiments of Kegel and Dhont [17] support this trend, although the final structure was the faulted-twinned fcc [18]. The metastability of the rhcp structure and stability of the fcc structure have been supported by numbers of experimental results [19, 20, 21, 22]. In addition to the reduction of the stacking disorder, these results also indicate that some stacking disorders remain at a late stage. The difference between the states at a late stage implies that the states observed are not in true equilibrium. Thus, the disappearance of defects in most cases must be a process between two metastable states. Though what this paper deals may be mere one of such processes, it should provide an insight into controlling defects. A recent remarkable experimental result, which supports the variety of the metastable states, is an small-angle X-ray diffraction study of silica colloids by Dolbnya *et al.* [23]. Their samples were aged for 1.5-2 years, which is in contract to those in previous studies: the times involved in the experiments of Zhu *et al.* were limited by the flight time of the Space Shuttle, although details were not described, and the aging times in the experiments of Kegel and Dhont were, at most, a few tens of days. It should be pointed out that [20] have presented a result, not reported in [15], that even under microgravity the fcc structure develops after thousands of seconds. Dolbnya *et al.* [23] have found a scattering pattern indicating a mostly complete fcc. Similar results have been obtained for a PMMA dispersion by a light scattering by Martellozzo *et al.* [21]. In opposition to the conclusion of Dolbnya *et al.* that melting of the rhcp structure followed by re-growth of fcc crystal is likely, we stress that this scenario is only one of the many processes possible. Despite that pre-melting near many types of defects, including the Shockley partial dislocation, has been observed [24] and supports this scenario, our opinion is that gradual disappearance of a defect, mediated by the motion of related defects, such as the glide of dislocation, cannot be ruled out.

The growth of a $\{111\}$ -oriented crystal occurs more often on a flat, bottom wall. This phenomenon can be understood through the orientational dependence of the interfacial free energy, which for an fcc HS crystal against a hard flat wall is lowest for a $\{111\}$ crystal orientation at the wall, compared with the other two common low-index orientations: $\{100\}$, and $\{110\}$ [25]. In the $\{111\}$ growth, however, stacking disorder can-

not be avoided for the reason discussed above; that is, the density is the same for any stacking sequences. For $\{100\}$ growth, on the other hand, the stacking sequence is unique. In a technique sometimes referred to as colloidal epitaxy, van Blaaderen *et al.* [26], used a template to force the crystal growth in the $\langle 001 \rangle$ direction. A patterned substrate [26, 27, 28, 29] or a substrate with a structure possessing the symmetry same as the $\{100\}$ face [30, 31, 32] must provide a stress as a driving force for the $\{100\}$ growth. Despite this bias toward $\{100\}$ growth, Schall *et al.* [33] used confocal microscopy to observe a stacking fault running along $\{111\}$ in the colloidal epitaxy of a PMMA suspension. This stacking fault was found to be terminated by the Sockley partial dislocation. Schall *et al.* interpret this as a misfit dislocation; thus, this structure is in equilibrium in the sense that the strain energy is minimized. In this paper, we stress that the same structure, which is in a metastable state, does disappear. One can say that the $\{001\}$ growth has an additional advantage that even if some excess stacking faults exist in a stage, some of them may disappear in a later stage through the mechanism we shall present in this paper. Again, the purpose of the paper is to provide a mechanism for the gradual disappearance of a defect. A detailed statistical analysis of this mechanism will be left to future research.

2 Simulation

In previous MC simulations [34], we observed the formation of a highly defective crystalline region above a well-ordered crystal at the bottom of a HS system under gravity. The structure of the highly defective crystalline region depends on the growth direction: For $\{100\}$ growth the highly defective region was observed to include several kinds of defects, whereas for the $\{111\}$ growth the defective region was smectic-like in appearance, and, upon closer examination, was observed to consist of layers with significant crystallinity. For the $\{100\}$ growth, we used a system size of $N = 1664$ particles contained in a box of dimensions $L_x=L_y=6.27\sigma$ and $L_z=49.2\sigma$. For the $\{111\}$ growth, $N = 3744$ particles were used with $L_x=L_y=9.40\sigma$ and $L_z=60.0\sigma$. Periodic boundary conditions were used in the x and y directions and well-separated hard walls were placed at $z = L_z$ (top) and $z = 0$ (bottom). We speculate that the observed $\{001\}$ growth results from stress due to the small system size and square symmetry in the horizontal (x and y) direc-

tions. This stress must play an similar role in the colloidal epitaxy [26, 27, 28, 29, 30, 31, 32, 33]. At least, the differences in the diagonal components of the strain from one another is of the same symmetry because, whereas the horizontal lattice spacing is fixed, the vertical one can vary [35].

In this study [34] the magnitude of the gravitational force was increased stepwise; the gravitational constant $g^* = mg\sigma/k_B T$ was increased by an increment $\Delta g^* = 0.1$ every 2×10^5 MC cycle (MCC) ($\Delta t = 2 \times 10^5$ MCC) up to a maximum value of $g^* = 1.5$. Here, m is the mass of a particle, T the temperature, and one MCC is defined by a set of N position moves. We remark that through this gradual stepwise increase of g^* we can successfully avoid metastable polycrystalline (we have suffered from these phenomena in an early stage of the study [36]) and glassy states. The effect that the gravity slows down the crystallization at high density has been observed by a MD simulation [37], in agreement with [36]. Also we note that the stepwise control can be efficiently realized by use of a centrifugation rotator [38, 39]. In earlier work, we reported that the formation of a less defective crystalline region started around $g^* = 0.9$; up to $g^* = 0.8$ the bottom of the system was occupied by a defective crystal [34]. We report here the behaviour of the system, which exhibited the (001) growth, focusing on the stacking faults.

3 Shrinking stacking fault

To illustrate the evolution of the system configuration for $g^* = 0.9$, we show in Fig. 1 (a)-(e), three-dimensional snapshots at 1.90, 1.92, 1.94, 1.96, and 1.98×10^6 MCC, respectively. The regions where disorder in stacking sequence occurs are marked with a red line except for Fig. 1 (a); we shall identify this disorder with an intrinsic stacking fault later. Based on these snapshots, we can conclude that shrinkage of an intrinsic stacking fault occurs in this system. In Fig. 1 (f) we plot the center of the gravity, z_G , which moves to lower positions as the simulation proceeds (though the ‘4ime’ average is not taken, the data is sufficient to show the trend). While the single stacking fault is shrinking, the velocity of decreasing of z_G is small. On the other hand, the sinking velocity is high when the conversion rate from the disordered to ordered states is high. In addition, we observe that the motion is not simply associated with the increasing height of the deficit region (as we shall see the lower end of an intrinsic stacking fault accompanies a particle deficiency as

shown in Fig. 3) in a viscous medium; the motion is better explained in terms of the elastic interaction between the defect and the strain field. In some cases buoyancy and elastic effects cooperate with each other to accelerate the motion. We have observed that the conversion of the defective crystal into an ordered crystal under gravity is caused by disappearance of stacking faults. In other words, we have successfully demonstrated the role of gravity reducing stacking faults. One point that should be noted is that the observations have been made over a relatively short period, along with a short simulation duration. We again note that there are many possible processes involved in the disappearance of defects and what we are observing here are those processes that take place at relatively short time scales. In addition, because the magnitude of Δt is not large, it follows that the stepwise control of the centrifugation rate is promising in a sense that the mechanism described in this paper must be of realizable time scale.

4 Shockley partial dislocation

Evolution of the particle configuration within the 18th to 21st layers from the bottom of the system is shown in Fig. 2. The projections of the configurations onto xy plane correspond approximately to a square lattice, indicating that the lattice planes are fcc (001) planes with the [110] and $[\bar{1}10]$ directed along the x and y directions. The shrinkage of the defect in Fig. 1 corresponds to the disappearance of regions where the square lattice is shifted by a half of its lattice constant, $a/\sqrt{2}$, where a is the fcc lattice constant ($a/\sqrt{2}$ is equal to the nearest-neighbour interparticle separation for an fcc crystal). In particular, disappearance of the defect is completed in the 18th layer at 1.94×10^6 th MCC and in the 19th layer at 1.96×10^6 th MCC. The magnitude of this shift is equal to the length of projection of the Burgers vectors of the Shockley partial dislocations onto the direction of the Burgers vector of the corresponding perfect dislocation. The translation of a fcc (111) plane along $[\bar{1}01]$ by one lattice constant, $a/\sqrt{2}$, of the triangular lattice of the (111) plane is decomposed into two motions: one of which translates particles in A-type sites onto B-type sites and the other in B-type to adjacent A-type [40]. Here, A and B refer to two of the three possible layer positions in projection onto the (111) plane (C refers to the last one). The translation vector \mathbf{b} , which is the Burgers vector of a perfect dislocation, for one interparticle spac-

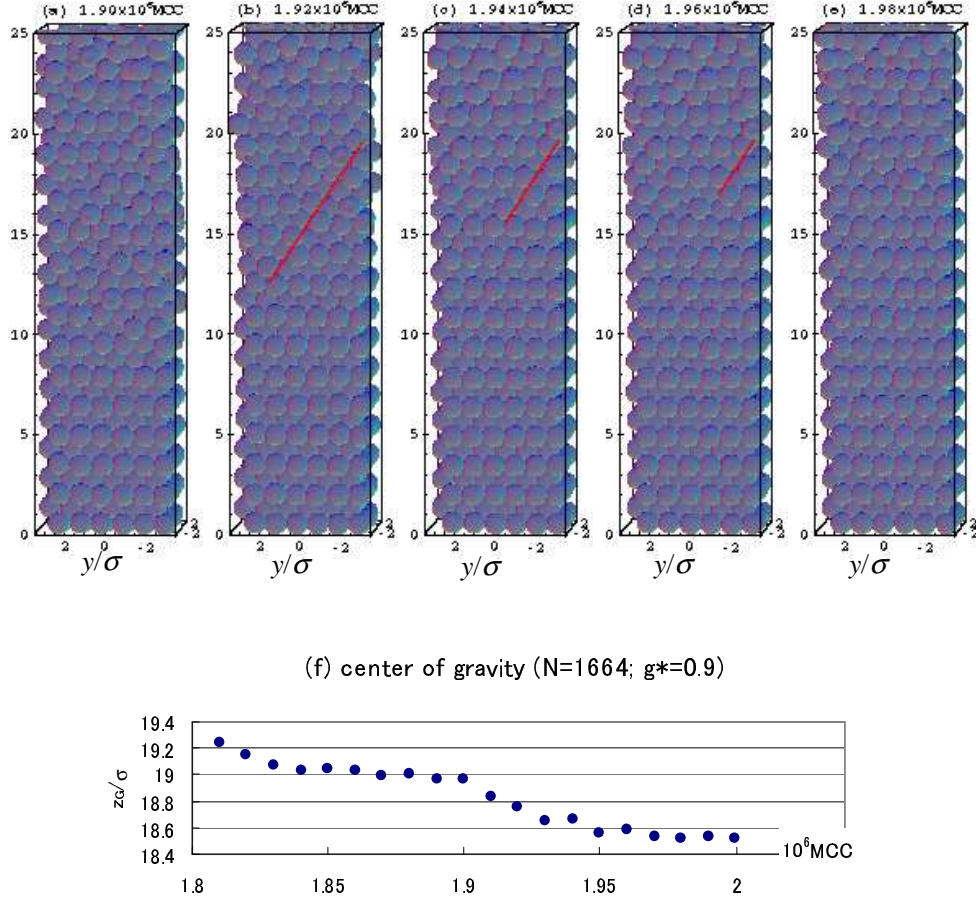


Figure 1: Evolution of particle configuration in three-dimensional view and the center of gravity. We show views from $-x$ direction at (a) 1.90 , (b) 1.92 , (c) 1.94 , (d) 1.96 , and (e) 1.98×10^6 th MCC. The red lines indicate a stacking fault, which is shrinking as simulation proceeds [The line is not drawn in (a) because the structure is complicated.] (f) the center of gravity, z_G , is plotted.

ing along $\langle 110 \rangle$ direction is decomposed into $\mathbf{b}^I + \mathbf{b}^{II}$, where \mathbf{b}^I and \mathbf{b}^{II} are the Burgers vectors of the Shockley partial dislocations. Translation by \mathbf{b}^I or \mathbf{b}^{II} also gives rise to the shift of lattice planes in the vertical direction that is shown in Fig. 3 - the blue (dashed) lines are shifted upward with respect to the green (dotted) lines. In Fig. 1 we examine a surface of the simulation box from $-x$ direction. The fcc unit cell is, thus, as illustrated in Fig. 4. The Burgers vectors are, respectively, $\mathbf{b} = (1/2)[110]$ ($=\mathbf{a}_1/2 + \mathbf{a}_2/2$ with \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 denoting the lattice vectors), $\mathbf{b}^I = (1/6)[211]$, and $\mathbf{b}^{II} = (1/6)[12\bar{1}]$; \mathbf{b}^I , which makes a shift of magnitude $a/2\sqrt{2}$ in the x direction in Fig. 2 and a shift of magnitude $a/6$ in the vertical direction in Fig. 3, is drawn by an arrow in Fig. 4. The difference in the magnitudes of the shifts in horizontal and vertical directions in Fig. 3 is affected by the differences in lattice constants in the vertical and horizontal directions due to the compression of the fcc unit cell in the ver-

tical direction [35]. In this way, we show that the region marked by blue (dashed) lines in Fig. 3 slides along $[211]$ direction. This operation yields an intrinsic stacking fault, i.e., stacking sequence such as ABCBCA... is made from ABCABC... In conclusion, an intrinsic stacking fault shrank through a glide of the Shockley partial dislocation. We note that the Frank partial dislocations, whose Burgers vector in the present case was $(1/3)[\bar{1}11]$, were not observed; if this had occurred the number of planes along $[\bar{1}11]$ would have varied across the Frank partial dislocation.

In addition to the stacking fault, we find deformation of the crystal; the crystal lattice in the defective region was twisted with respect to the bottom-ordered lattice as shown in Fig. 2 and the lattice planes were inclined with respect to the bottom-ordered crystal as shown in Fig. 3. Twist and tilt boundaries are anticipated along the horizontal direction. Comparing the 19th and 20th layers in

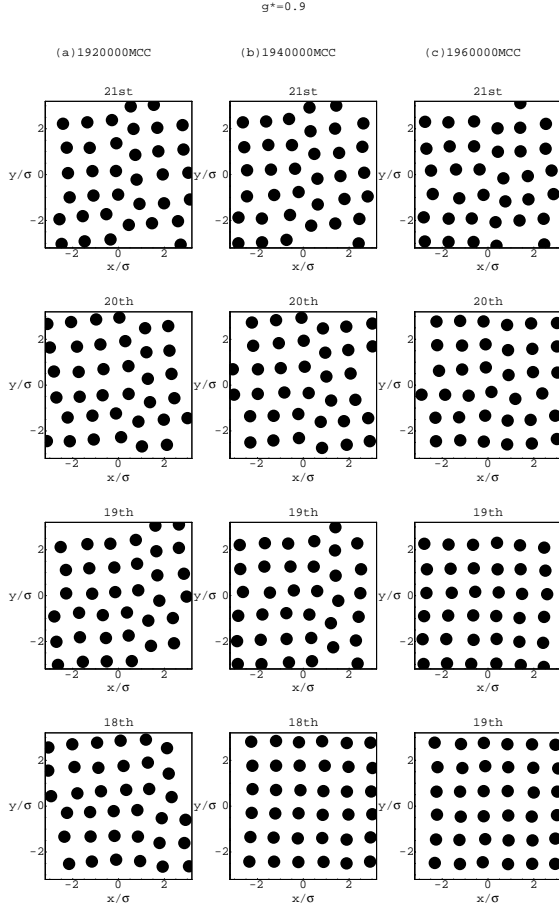


Figure 2: Evolution of particle configuration of several crystalline layers. We plot particle positions in 18th to 21st layers from the bottom of the system at (a) 1.92 , (b) 1.94 , and (c) 1.96×10^6 th MCC. The z coordinate of each layer can be taken from Fig. 3.

Fig. 2 (c) with those in Figs. 2 (a) and (b) the twist is found to disappear as the stacking fault disappears. Also, we see the simultaneous disappearance of the inclination. Taking a close look at Fig. 3 we see that, due to the inclination of the lattice planes, the right side and left sides of a lattice plane appear to match up with each other across the periodic boundary. This means that, for instance, the B-type ($\bar{1}11$) plane gradually changes to the A-type ($\bar{1}\bar{1}1$) plane. It follows that strain energy is released during the process of stacking fault disappearance. Of course, there is a density increase corresponding to the translation of lattice planes downward. It is conjectured that the cooperation of those effects makes the disappearance of stacking faults at a condition with $g^*=0.9$; this condition can be rewritten

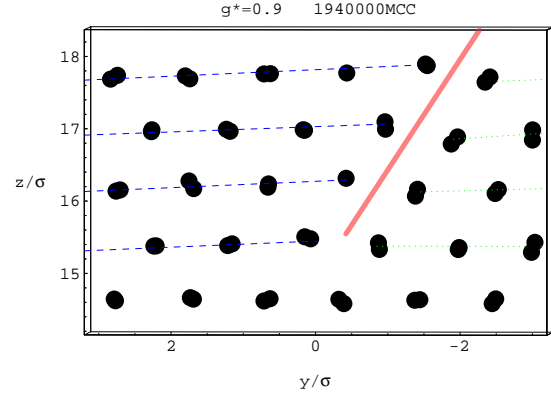


Figure 3: Side view of crystalline layers: 18th to 22nd layers are from the bottom. The region $-2.92 < x/\sigma < -0.92$ at 1.94×10^6 th MCC is viewed from $-x$ direction; a few layers from the surface are shown to avoid complication. Dashed (blue) and dotted (green) lines, drawn for guide of viewing, indicate the slide of dashed (blue) region occurs along the thick (red) line.

ten so that the gravitational length $l_g = k_B T / mg$ is slightly greater than the HS diameter σ .

We should add a remark with regard to the strain. The interlayer spacing varies along the vertical direction whereas the interparticle separation in a layer does not vary appreciably [35], so non-uniform uniaxial compression is observed. However, the relief of twist and tilt must lower the system free energy irrespective of the existence of non-uniform uniaxial compression. In our opinion, the defects in colloidal crystals can be controlled through the mechanisms found by this MC simulation. We note the effect of system size on the inclination of a layer; in contrast to the twists, stress due to the inclination may decrease with increasing system size as the inclination angle becomes small or matches that corresponding to the periodicity of the “dislocation” array that minimizes the strain energy.

5 Conclusion and remarks

We have successfully demonstrated the disappearance of a stacking fault for (001) growth in a hard-sphere fcc crystal under gravity. In other words, we have given an answer to the speculation that stacking faults are reduced under gravity [15]. While an intrinsic stacking fault is terminated by the Shockley partial dislocation at an end, traversing the system horizontally the translation gradually disappears in a plane through the gradual variation of

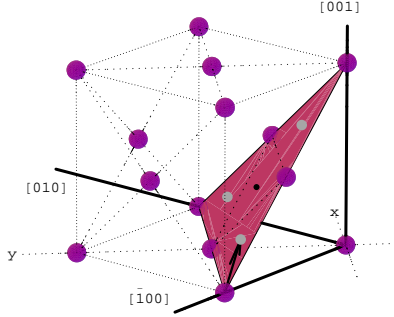


Figure 4: Figure 4 Schematic figure of translation corresponding to the Shockley partial dislocation. The $(\bar{1}11)$ plane is marked (painted in red). The Burgers vector of the Shockley partial dislocation, $\mathbf{b}^I = (1/6) [211] = \mathbf{a}_1/3 + \mathbf{a}_2/6 + \mathbf{a}_3/6$, is shown by an arrow. Here, lattice vectors are denoted as \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 . We see that \mathbf{b}^I makes shifts of magnitude $a/2\sqrt{2}$, $a/6\sqrt{2}$, and $a/6$, respectively, along $[110]$, $[1\bar{1}0]$, and $[001]$.

the magnitude of inclination of a (001) layer. In addition, we observe the existence of twists of portions of a (001) plane with respect to the bottom-ordered crystal. Those crystal deformations that disappear during shrinkage of a stacking fault do so via a glide of the Shockley partial dislocation. The disappearances of twist and tilt boundaries as well as of the deformations are considered to lower the system free energy. The density increase, which accompanies the decrease of the gravitational energy during the shrinkage of stacking faults, has a tendency to cooperate with those phenomena.

In this paper, we have provided some intuition into the gravity-induced disappearance of stacking faults in a hard-sphere crystal, while avoiding a detailed statistical analyses employing strain-energy formulae and numerics. A strain-energy formulation for the present defect configuration, such as described in [40], is in progress [41]. On the other hand, some of parameters necessary for accurate numerical evaluation are lacking [namely, the dislocation core energy and the density dependence of the stacking fault free energy ** in the strongly inhomogeneous case, such as in the high- g^* regime (note that the pressure gradient, $\partial P/\partial z$, equals

** The interfacial free energy of stacking fault calculated near the crystal-fluid phase transition [12] is of order $10^{-4} k_B T$ per unit area, so the interfacial energy contributes less as compared with the strain energy.

$-mg\rho(z)$ with $\rho(z)$ being the particle number density]). We present the result in this style, with the strain energy calculation being left at the future research, is because the strain illustrated in the present figures evidently contribute dominantly; the energy of such strain field logarithmically depends on the linear dimension over which the field extends.

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